**Syllabus Chem 560 module on analysis of dynamic systems (2017) (CRN TBD)**

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*1. Lectures*

- The class will mainly consist of be 9–11 hours of lectures, delivered as described on the website. Student-delivered lessons will account for another ~2 hours.

*2. Student presentations on related techniques*

- Each student will be assigned a related technique (not NMR), and will be responsible for presenting to the class an in-depth lesson on using that technique for studying dynamic systems.

- Each lesson will last 30 minutes, and should include at least:

Background and instrumentation

Theory of the method

The mathematics of determining Kassocor other important parameters

Case studies

Errors, assumptions, limitations

This is a free-form lesson for you to control. The format of delivery (powerpoint, chalkboard, or whatever) is to be decided by each student. Grading of your presentation will be weighted as: 40% visual aids / 40% content / 20% presentation style and overall impression.

*3. Final exam.*

- Time and Date to be determined.

- The lessons delivered by the other students are testable material.

- Practice problems will be distributed.

**Evaluation**

Student presentation: 40%

Attendance, participation in discussion, and practical NMR titration assignment: 20%

Final exam: 40%

**Reference material**

*Supramolecular chemistry (2nd edition)*, J.W. Steed and J.L. Atwood, John Wiley and sons, Chichester, 2009.

*Binding constants. The measurement of molecular complex stability.* K.A. Connors, John Wiley and sons, Toronto, 1987.

*Analytical Methods in Supramolecular Chemistry*, Edited by C. Schalley, Wiley-VCH.

**List of topics**

***A. Intro to dynamic systems***

1. The association constant: Kassoc

2. Thermodynamic parameters: ∆G, ∆H, ∆S

3. Rate constants (k1 = kon, k–1 = koff)

4. Weak interactions: a) electrostatics, b) dispersion, c) hydrogen bonds, d) aromatic interactions, e) cation-pi, f) halogen bonds, g) hydrophobic effect

***B. Stoichiometry and Kassoc by NMR***

1. NMR of free and bound states and the NMR time scale

2. Determining complex stoichiometries

2a. Heteromeric assemblies: stoichiometry by integration

2b. The method of continuous variation (Job plot).

2c. Stoichiometry by Diffusion Ordered SpectroscopY (DOSY-NMR)

2d. Other methods for determining solution stoichiometry

3. Determining Kassoc for systems in slow exchange

4. Determining Kassoc for systems in fast exchange

4a. A special case: when ∂free and ∂bound are known

4b. The normal case: when ∂bound is unknown — titrations

The 1:1 binding isotherm

Method 1. Linearized plots

Method 2. Non-linear plot and curve fitting

5. How to run and analyze an NMR titration

***C. Thermodynamic parameters by NMR***

van’t Hoff plots, assumptions and errors

***D. Exchange kinetics by NMR***

Case 1. Very slow kinetics.

Case 2. Intermediate exchange kinetics. NMR line-shape analysis.

Case 3. Slow-to-intermediate exchange kinetics. The EXSY experiment.

***E. Other techniques — Student presentations***

UV-Vis —

Fluorescence —

Fluorescence Polarization —

Homodimerization studies —

Numerical solutions for Chemical Equilibria —

Potentiometry —

Patch clamp analyses —

Isothermal Titration Calorimetry —

Extraction/partition experiments —

Surface Plasmon Resonance (SPR/Biacore) —

Other biochemical methods… Alpha Screen, ELISA, TR-FRET, etc.

… and any others that you might suggest, as long as they are pre-approved by Dr. Hof.